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INTERFACES DESIGNED ATOM BY ATOM AND NANOMETER BY NANOMETER TO OPTIMIZE CHARGE TRANSFER IN ENERGY CONVERSION*

The performance of energy conversion and storage devices such as batteries, fuel cells, electrolyzers, photoelectrochemical cells, and solar cells is determined to a large extent by the ease with which charge carriers are transferred across the interface between two phases and transported towards the interface (and away from it). Therefore, engineering the interface in terms of both its geometry and its physical-chemical properties represents the prime method for optimizing the performance of energy conversion devices — if the fundamental steps involved are well understood.

We address this challenge with a general preparative strategy based on a highly ordered nanoporous template and a highly conformal coating method. We make templates consisting of straight, cylindrical pores in hexagonally arranged arrays by an electrochemical procedure, anodization. The pores' diameter can be set to values between 20 nm and 400 nm, their length between 100 nm and 100 μm. We coat the inner walls of the pores by atomic layer deposition (ALD), a chemical method that allows for the generation of thin films from molecular (gaseous or dissolved) precursors even in structured substrates. The thickness of these functional coatings can be adjusted between 0.2 nm and 50 nm. Together, anodization and ALD provide the opportunity to prepare nearly perfect model systems in which to study systematically how charge transport to an interface and charge transfer across it can be affected by the nanoscale geometry of the interface.

In the field of water electrolysis, these methods have enabled us to minimize the loading of noble metal catalysts to very low values below 10 μg/cm^2. If abundant but catalytically less active transition metal oxides are used, the pores can be elongated in order to increase surface area, and thereby electrocatalytic turnover, until transport in the electrolyte becomes limiting. In photovoltaic systems based on the "extremely thin absorber" concept and abundant, non-toxic elements, ALD has allowed for the accurate tuning of a tunnel barrier that prevents the undesired recombination of charge carriers with an optimized thickness of 1.0 nm. The coaxial nanocylindrical geometry obtained in parallel nanopore arrays has enabled us to achieve state-of-the-art efficiencies with reduced amount of material as compared with established systems based on disordered mesoporous layers (Fig. 1).

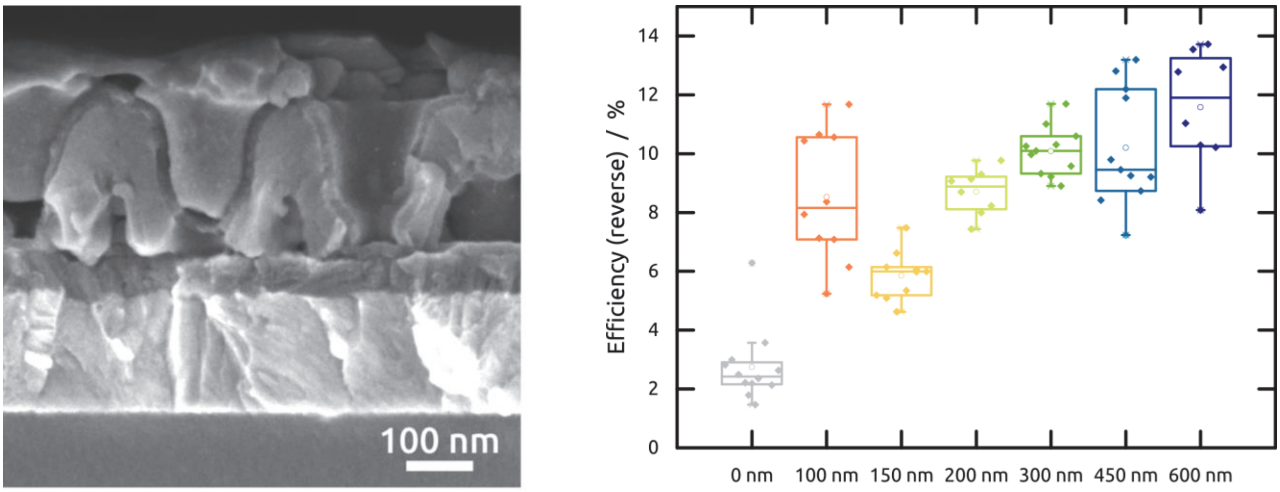

Fig. 1. Characterization of solar cells based on ordered arrays of coaxial nanocylindrical semiconductor junctions: left, scanning electron micrograph in cross-section; right, performance dependence on the cylinder length

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